



Atom Bond Connectivity Indices of Kragujevac Trees (Kgd,k)

Keerthi G. Mirajkar¹, Bhagyashri R. Doddamani², Priyanka Y.B.³

^{1,2,3}Department of Mathematics, Karnatak University's Karnatak Arts College, Dharwad - 580001, India.

ABSTRACT

Aim: The aim of this article is to determine first four types of atom bond connectivity indices of Kragujevac trees with isomorphic branches and increased ordered branches.

Methodology: The method applied to obtain the goal of this article is analytic.

Results: The results we constructed here are for first four types of atom bond connectivity indices of Kragujevac tree with all branches of tree are mutually isomorphic to each other and increasing ordered branches.

Conclusion: The first four types of atom bond connectivity indices on kragujevac trees with isomorphic branches and increasing ordered branches are determined. Also, atom bond connectivity indices can be computed for other class of graphs.

Key Words: Atom bond connectivity indices, Kragujevac tree

AMS Subject classification: 05C05, 05C07, 05C12

INTRODUCTION

Mathematical chemistry is a branch of theoretical chemistry using mathematical methods to discuss and predict molecular properties without necessarily referring to quantum mechanics [1,15,22]. Chemical graph theory is a branch of mathematical chemistry which applies graph theory in mathematical modeling of chemical phenomena [8]. This theory has an important effect on the development of the chemical sciences.

A graph $G = (V, E)$ is a collection of points and lines connecting them. The points and lines of a graph are also called vertices and edges respectively. If e is an edge of G , connecting to the vertices u and v , then we write $e = uv$. A connected graph is a graph such that there exists a path between all pairs of vertices. The distance $d(u, v) = d_G(u, v)$ between two vertices u and v is the length of the shortest path between u and v in G .

A molecular graph is a simple graph such that its vertices correspond to the atoms and edges corresponds to the bonds. According to the IUPAC terminology, a topological index is a numerical value associated with chemical constitution, which can be then used for correlation of chemical structure

with various physical and chemical properties, chemical reactivity and biological activity [9,10,12,17,19,20,21,24].

In mathematical chemistry, numbers encoding certain structural features of organic molecules and derived from the corresponding molecular graph, are called graph invariants or more commonly called as topological indices.

Among topological descriptors, connectivity indices are very important and they have a prominent role in chemistry. In other words, if G be the connected graph, then we can introduce many connectivity topological indices for it, by distinct and different definition.

One of the best known and widely used is the connectivity index, introduced in 2009, Furtule[4] proposed the first atom bond connectivity index of a graph G as:

$$ABC_1(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \quad (1)$$

Where d_u denotes degree of vertex u and d_v denotes degree of vertex v in G .

The second atom bond connectivity index is introduced by A. Graovac[7]. It is defined as follows:

Corresponding Author:

Keerthi G. Mirajkar, Assistant Professor, Dep of Mathematics, Karnatak University's Karnatak Arts College, Dharwad, Karnataka, India - 580001, Contact No. 9945526640; E-mail: keerthi.mirajkar@gmail.com

ISSN: 2231-2196 (Print)

ISSN: 0975-5241 (Online)

DOI: 10.7324/IJCRR.2017.9151

Received: 27.05.2017

Revised: 14.06.2017

Accepted: 10.07.2017

$$ABC_2(G) = \sum_{uv \in E(G)} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}} \quad (2)$$

Where n_u denotes the number of vertices of G whose distance to the vertex u is smaller than distance to the vertex v .

Farahani[3] proposed a third atom bond connectivity index of G as follows:

$$ABC_3(G) = \sum_{uv \in E(G)} \sqrt{\frac{m_u + m_v - 2}{m_u m_v}} \quad (3)$$

where m_u is the number of edges of G lying closer to u than to v and m_v is the number of edges of G lying closer to v than to u .

Ghorbani [6] defines a new version of atom bond connectivity index. It is named as fourth atom bond connectivity index and defined as:

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{s_u + s_v - 2}{s_u s_v}} \quad (4)$$

where s_u denotes the sum of degrees of all neighbor of vertex u in G . Reader can find the history and results on this family of indices in [23,25-27].

All graphs considered here are connected, finite without multiple edges and loops. For undefined terminologies, we refer to [16].

Motivated by [3,4,6,7], In this article we study and compute the above mentioned four types of Atom Bond Connectivity Indices on the special class of graph called the Kragujevac tree with isomorphic branches and increasing ordered branches.

Definition 2.1. [11] Let P_3 be the 3 vertex tree rooted at one of its terminal vertices, see Figure 1. For $k = 2, 3, \dots$ construct the rooted tree B_k by identifying the roots of k copies of P_3 . The vertex obtained by identifying the roots of P_3 trees is the root of B_k .

Examples illustrating the structure of the rooted tree B_k are depicted in Figure.1.

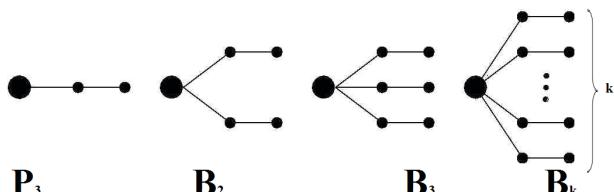


Figure 1

The rooted trees B_2 , B_3 and B_k obtained respectively by identifying the roots of 2, 3 and k copies of P_3 . Their roots are

indicated by large dots.

Definition 2.2. [11] Let $d \geq 2$ be an integer. Let $\beta_1, \beta_2, \dots, \beta_d$ be rooted trees specified in definition 2.1, i.e., $\beta_1, \beta_2, \dots, \beta_d \in \{B_2, B_3, \dots\}$. A Kragujevac tree T is a tree possessing a vertex of degree d , adjacent to the roots of $\beta_1, \beta_2, \dots, \beta_d$. This vertex is said to be the central vertex of T where as d is the degree of T . The subgraphs $\beta_1, \beta_2, \dots, \beta_d$ are the branches of T . Recall that some (or all) branches of T may be mutually isomorphic. A typical kragujevac tree is depicted in Figure.2.

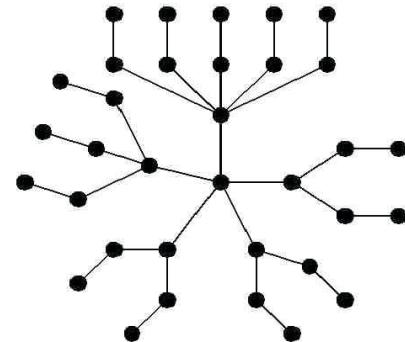


Figure 2.

A Kragujevac tree of degree $d = 5$, in which $\beta_1, \beta_2, \beta_3 \cong B_2, \beta_4 \cong B_3, \beta_5 \cong B_5$. The branches B_k has $2k + 1$ vertices and $2k$ edges. A typical Kragujevac tree is denoted by $Kg_{d,k}$ where $d \geq 2$ is the degree of central vertex and $k \geq 2$.

Methodology:

In this article, we determine the first four types of atom bond connectivity indices on a special class of graph called as Kragujevac tree. To find these four types of atom bond connectivity indices on Kragujevac tree we have applied analytic method and hence established the following results.

RESULTS

Theorem 3.1. Let $Kg_{d,k}$ be the Kragujevac tree of degree $d \geq 2$ with all branches B_k of tree are mutually isomorphic to each other. Then the first atom bond connectivity of $Kg_{d,k}$

$$ABC_1[Kg_{d,k}] = 2(kd) \sqrt{\frac{1}{2} + d} \sqrt{\frac{d+k-1}{d(k+1)}}$$

Proof. By the definition of kragujevac tree $Kg_{d,k}$ of degree $d \geq 2$, with all isomorphic branches $B_k, \forall k \geq 2$. Further each branch B_k of $Kg_{d,k}$ contains k pendent vertices. Then the kragujevac tree contains $[k(2k+1) + 1]$ vertices and $(2k+d)$ edges.

We consider the following cases to compute the proof, which are depending upon the degree of the vertices in $Kg_{d,k}$.

Case i. Each branch B_k has $2k$ edges, where k edges are incident with pendent vertices and the vertices of degree 2. Remaining k edges are incident with vertices of degree 2 and vertex of degree $(k+1)$. Since there are d number of branches present in $Kg_{d,k}$, then

From equation (1),

The ABC_1 for d number of B_k branches of $Kg_{d,k}$ is

$$ABC_1 = d \left[2k \sqrt{\frac{1}{2}} \right] \quad (5)$$

Case ii. Now consider the d edges incident with central vertex of degree d and the vertices of degree $(k+1)$.

From equation (1),

The ABC_1 for d edges of $Kg_{d,k}$ is

$$ABC_1 = d \sqrt{\frac{d+k-1}{d(k+1)}} \quad (6)$$

From equation (5) and (6),

$$ABC_1[Kg_{d,k}] = 2(kd) \sqrt{\frac{1}{2}} + d \sqrt{\frac{d+k-1}{d(k+1)}}$$

Corollary 3.2. The first atom bond connectivity of Kragujevac tree $Kg_{d,k}$, when $d = k$ is

$$ABC_1[Kg_{d,k}] = 2k^2 \sqrt{\frac{1}{2}} + k \sqrt{\frac{2k-1}{k(k+1)}}$$

Proof. The proof follows from the theorem 3.1 and replacing d by k

Theorem 3.3. Let $Kg_{d,k}$ be the Kragujevac tree of degree $d \geq 2$ with all branches B_k of tree are mutually isomorphic to each other, then the second atom bond connectivity of $Kg_{d,k}$ is

$$ABC_2[Kg_{d,k}] = d \left[k \left(\sqrt{1 - \frac{1}{d(2k+1)}} + \sqrt{\frac{1}{2}} \right) + \sqrt{\frac{d(2k+1)-1}{(2k+1)[2k(d-1)+d]}} \right]$$

Proof. Here we consider the Kragujevac tree $Kg_{d,k}$ of degree $d \geq 2$, with all isomorphic branches $B_k, \forall k \geq 2$. We compute the ABC_2 by considering the following cases depending upon the distance between the vertices in $Kg_{d,k}$.

Case i. Each branch B_k has $2k$ edges, where k edges are incident with pendent vertices and the vertices of degree 2. Here one vertex of degree 2 is closer to the pendent vertices and $[d(2k+1)]$ vertices are closer to the vertices of degree 2. The remaining k edges are incident with vertices of degree 2 and vertex of degree $(k+1)$. Hence 2 vertices are closer to vertices of degree 2 and $[d(2k+1)-1]$ edges are closer to the vertex of degree $(k+1)$. Since there are d number of branches present in $Kg_{d,k}$, then

branches present in $Kg_{d,k}$, then

From equation (2),

The ABC_2 for d number of B_k branches of $Kg_{d,k}$ is

$$ABC_2 = d \left[k \sqrt{1 - \frac{1}{d(2k+1)}} + k \sqrt{\frac{1}{2}} \right] \quad (7)$$

Case ii. Now consider the d edges incident with central vertex of degree d and the vertices of degree $(k+1)$. Here the $(2k+1)$ vertices are closer to the vertices of degree $(k+1)$ and $[d(2k+1)-2k]$ vertices are closer to the vertex of degree d .

From equation (2), The ABC_2 for d edges of $Kg_{d,k}$ is

$$ABC_2 = d \sqrt{\frac{d(2k+1)-1}{(2k+1)[2k(d-1)+d]}} \quad (8)$$

From equation (7) and (8),

Corollary 3.4. The second atom bond connectivity of Kragujevac tree $Kg_{d,k}$, when $d = k$ is

$$ABC_2[Kg_{d,k}] = d \left[k \left(\sqrt{1 - \frac{1}{d(2k+1)}} + \sqrt{\frac{1}{2}} \right) + \sqrt{\frac{d(2k+1)-1}{(2k+1)[2k(d-1)+d]}} \right]$$

Proof. The proof follows from the theorem 3.3 and replacing d by k .

Theorem 3.5. Let $Kg_{d,k}$ be the Kragujevac tree of degree $d \geq 2$ with all branches B_k of tree are mutually isomorphic to each other. Then the third atom bond connectivity of $Kg_{d,k}$ is

$$ABC_3[Kg_{d,k}] = d \left[k \left(\sqrt{1 - \frac{1}{d(2k+1)}} + \sqrt{\frac{1}{2}} \right) + \sqrt{\frac{d(2k+1)-1}{(2k+1)[2k(d-1)+d]}} \right]$$

Proof. Here we consider the Kragujevac tree of degree $d \geq 2$, with all isomorphic branches $B_k, \forall k \geq 2$. We consider the following cases to compute the proof, which are depending upon the distance between of the edges and vertices in $Kg_{d,k}$.

Case i. Each branch B_k has $2k$ edges, where k edges are incident with pendent vertices and the vertices of degree 2. Here one edge is closer to the pendent vertices and $[d(2k+1)]$ edges are closer to the vertices of degree 2. The remaining k edges are incident with vertices of degree 2 and vertex of degree $(k+1)$. Hence 2 edges are closer to vertices of degree 2 and $[d(2k+1)-1]$ edges are closer to the vertex of degree $(k+1)$. Since there are d number of branches present in $Kg_{d,k}$, then

From equation (3),

The ABC_3 for d number of B_k branches of $Kg_{d,k}$ is

$$ABC_3 = d \left[k \sqrt{1 - \frac{1}{d(2k+1)}} + k \sqrt{\frac{1}{2}} \right] \quad (9)$$

Case ii. Now consider the d edges incident with central vertex of degree d and the vertices of degree $(k+1)$. Here $(2k+1)$ edges are closer to the vertices of degree $(k+1)$ and $[d(2k+1)-2k]$ edges are closer to the vertex of degree d .

From equation (3),

The ABC_3 for d edges of $Kg_{d,k}$ is

$$ABC_3 = d \sqrt{\frac{d(2k+1)-1}{(2k+1)[2k(d-1)+d]}} \quad (10)$$

From equation (9) and (10),

$$ABC_3(Kg_{d,k}) = d \left[k \left(\sqrt{1 - \frac{1}{d(2k+1)}} + \sqrt{\frac{1}{2}} \right) + \sqrt{\frac{d(2k+1)-1}{(2k+1)[2k(d-1)+d]}} \right]$$

Corollary 3.6. The third atom bond connectivity of Kragujevac tree $Kg_{d,k}$, when $d=k$ is

$$ABC_3(Kg_{d,k}) = k^2 \left[\sqrt{1 - \frac{1}{k(2k+1)}} + \sqrt{\frac{1}{2}} \right] + k \sqrt{\frac{k(2k+1)-1}{k[(2k)^2-1]}}$$

Proof. The proof follows from the theorem 3.5 and replacing d by k .

Theorem 3.7. Let $Kg_{d,k}$ be the Kragujevac tree of degree $d \geq 2$, with all branches B_k of tree are mutually isomorphic to each other, then the fourth atom bond connectivity of $Kg_{d,k}$ is

$$ABC_4[Kg_{d,k}] = d \left[k \left(\sqrt{\frac{3k+d}{(k+2)(2k+d)}} + \sqrt{\frac{1}{2}} \right) + \sqrt{\frac{2(k+d-1)+dk}{d(k+1)(d+2k)}} \right]$$

Proof. Let $Kg_{d,k}$ be the Kragujevac tree of degree $d \geq 2$, with all isomorphic branches $B_k, \forall k \geq 2$. We consider the following cases to compute the proof, which are depending upon the degree of neighbor vertices of $Kg_{d,k}$.

Case i. Each branch B_k has $2k$ edges, where k edges are incident with pendent vertices and the vertices of degree 2. For the pendent vertices the neighbor vertices are of degree 2 and for the vertices of degree 2 the neighbor vertices are of degree $(k+2)$. The remaining k edges are incident with vertices of degree 2 and vertex of degree $(k+1)$. For the vertices of degree 2 the neighbor vertices are of degree $(k+2)$ and for the vertices of degree $(k+1)$ the neighbor vertices are of degree $(2k+d)$. Since there are d number of branches present in $Kg_{d,k}$, then

From equation (4),

$$ABC_4 = d \left[k \left(\sqrt{\frac{3k+d}{(k+2)(2k+d)}} + \sqrt{\frac{1}{2}} \right) \right] \quad (11)$$

Case ii. Now consider the d edges of $Kg_{d,k}$ which are incident with central vertex of degree d and the vertices of degree $(k+1)$. For the vertex of degree d the neighbor vertices are of degree $[d(k+1)]$ and for the vertices of degree $(k+1)$ the neighbor vertices are of degree $(2k+d)$.

From equation (4),

The ABC_4 for d edges of $Kg_{d,k}$ is

$$ABC_4 = d \sqrt{\frac{2(k+d-1)+dk}{d(k+1)(2k+d)}} \quad (12)$$

From (11) and (12),

$$ABC_4[Kg_{d,k}] = d \left[k \left(\sqrt{\frac{3k+d}{(k+2)(2k+d)}} + \sqrt{\frac{1}{2}} \right) + \sqrt{\frac{2(k+d-1)+dk}{d(k+1)(d+2k)}} \right]$$

Corollary 3.8. The fourth atom bond connectivity of Kragujevac tree $Kg_{d,k}$, when $d=k$ is

$$ABC_4[Kg_{d,k}] = k^2 \left(\sqrt{\frac{4k}{3k(k+2)}} + \sqrt{\frac{1}{2}} \right) + k \sqrt{\frac{2(2k-1)+k^2}{3k^2(k+1)}}$$

Proof. The proof follows from the theorem 3.7 and replacing d by k .

Remark 3.9. Let $Kg_{d,k}$ be the Kragujevac tree, $d \geq 2$ with branches $B_k, \forall k = 2, 3, \dots$, i.e. $\beta_1, \beta_2, \dots, \beta_d \in B_{i+1}, B_{i+2}, \dots, B_{i+n}, \forall i = 1, 2, 3, \dots$, respectively. i.e., with increasing ordered branches contains $(2[(i+1)+(i+2)+\dots+(i+n)]+d+1)$ vertices and $(2[(i+1)+(i+2)+\dots+(i+n)]+d)$ edges.

Theorem 3.10. Let $Kg_{d,k}$ be the Kragujevac tree of degree $d \geq 2$, with branches B_k and $\beta_1, \beta_2, \dots, \beta_d \in B_{i+1}, B_{i+2}, \dots, B_{i+n}, \forall i = 1, 2, 3, \dots$, respectively. Then the first atom bond connectivity for $Kg_{d,k}$ is

$$ABC_1[Kg_{d,k}] = \sum_{i=2}^n 2i \sqrt{\frac{1}{2}} + \sum_{i=2}^n \sqrt{\frac{d+i-1}{d(i+1)}}$$

Proof. Let $Kg_{d,k}$ be the Kragujevac tree of degree $d \geq 2$, with branches $B_k, \forall k = 2, 3, \dots$, we consider here in particular rooted trees $[\beta_1, \beta_2, \dots, \beta_d]$ of the type $B_{i+1}, B_{i+2}, \dots, B_{i+n}, \forall i = 1, 2, 3, \dots$, respectively. We consider the following cases to compute the ABC_1 of $Kg_{d,k}$.

Case i. By Remark 3.9, the branches $B_{i+1}, B_{i+2}, \dots, B_{i+n}$ has $(2[(i+1)+(i+2)+\dots+(i+n)])$ edges. In that $[(i+1)+(i+2)+\dots+(i+n)]$ edges are incident with pendent vertices and vertices of degree 2. The remaining $[(i+1)+(i+2)+\dots+(i+n)]$ edges are incident with vertices of degree 2 and vertices of degree $[(i+1)+1, (i+2)+1, \dots, (i+n)+1]$ respectively.

From equation (1),

$$ABC_1 = 2[(i+1)+(i+2)+\dots+(i+n)] \sqrt{\frac{1}{2}} \quad (13)$$

Case ii. Now consider the remaining d edges which are incident with vertex of degree d and the vertices of degree $\{(i+1)+1, (i+2)+1, \dots, (i+n)+1\}$ belongs to the branches $B_{i+1}, B_{i+2}, \dots, B_{i+n}$ respectively.

From equation (1),

$$ABC_1 = \sum_{i=2}^n \sqrt{\frac{d+i-1}{d(i+1)}} \quad (14)$$

From (13) and (14),

$$ABC_1[K_{d,k}] = \sum_{i=2}^n 2i \sqrt{\frac{1}{2}} + \sum_{i=2}^n \sqrt{\frac{d+i-1}{d(i+1)}}$$

Theorem 3.11. Let $Kg_{d,k}$ be the Kragujevac tree of degree $d \geq 2$, with branches B_k and the rooted trees $\beta_1, \beta_2, \dots, \beta_d \in B_{i+1}, B_{i+2}, \dots, B_{i+n}, \forall i = 1, 2, 3, \dots$, respectively. Then the second atom bond connectivity for $Kg_{d,k}$ is

$$ABC_2[Kg_{d,k}] = \sum_{i=2}^n \left(i \left[\sqrt{\frac{\sum_{i=2}^n 2i+d-1}{\sum_{i=2}^n 2i+d}} + \sqrt{\frac{1}{2}} \right] + \sqrt{\frac{\sum_{i=2}^n 2i+d-1}{(2i+1)[(\sum_{i=2}^n 2i)+d-2i]}} \right)$$

Proof. Let $Kg_{d,k}$ be the Kragujevac tree of degree $d \geq 2$, with branches $B_k, \forall k = 2, 3, \dots$ we consider here in particular rooted trees $[\beta_1, \beta_2, \dots, \beta_d]$ of the type $B_{i+1}, B_{i+2}, \dots, B_{i+n}, \forall i = 1, 2, 3, \dots$, respectively.

We discuss the following cases to construct the ABC_2 of $Kg_{d,k}$.

Case i. By Remark 3.9, the branches $B_{i+1}, B_{i+2}, \dots, B_{i+n}$ has $(2[(i+1)+(i+2)+\dots+(i+n)])$ edges. In that $[(i+1)+(i+2)+\dots+(i+n)]$ edges are incident with pendent vertices and vertices of degree 2. Further one vertex is closer to the pendent vertices and $(2[(i+1)+(i+2)+\dots+(i+n)]+d)$ vertices are closer to the vertices of degree 2.

Case ii. The remaining $[(i+1)+(i+2)+\dots+(i+n)]$ edges of branch B_k are incident with vertices of degree 2 and vertices of degree $[(i+1)+1, (i+2)+1, \dots, (i+n)+1]$ respectively. Further 2 vertices are closer to the vertices of degree 2 and $(2[(i+1)+(i+2)+\dots+(i+n)]+d-1)$ vertices are closer to the vertices of degree $[(i+1)+1, (i+2)+1, \dots, (i+n)+1]$.

From equation (2),

$$ABC_2 = \sum_{i=2}^n i \left[\sqrt{\frac{\sum_{i=2}^n 2i+d-1}{\sum_{i=2}^n 2i+d}} + \sqrt{\frac{1}{2}} \right] \quad (15)$$

Case iii. Now consider the remaining d edges of $Kg_{d,k}$ which are incident with vertex of degree d and the vertices of degree $[(i+1)+1, (i+2)+1, \dots, (i+n)+1]$ belongs to the branches $B_{i+1}, B_{i+2}, \dots, B_{i+n}$ respectively. Also $(2i+1), (2i+2), \dots, (2i+n)$ vertices are closer to the vertices of degree $(i+1)+1, (i+2)+1, \dots, (i+n)+1$ respectively and $(\sum_{i=2}^n 2i)+d-2(i+1) (\sum_{i=2}^n 2i)+d-2(i+2) \dots, (\sum_{i=2}^n 2i)+d-2(i+n)$ vertices are

closer to the vertex of degree d , when the vertex of degree d is adjacent with vertices of degree $(i+1)+1, (i+2)+1, \dots, (i+n)+1$ respectively.

From equation (2),

$$ABC_2 = \sum_{i=2}^n \sqrt{\frac{\sum_{i=2}^n (2i)+d-1}{(2i+1)[(\sum_{i=2}^n 2i)+d-2i]}} \quad (16)$$

From (15) and (16),

$$ABC_2[Kg_{d,k}] = \sum_{i=2}^n i \left[\sqrt{\frac{\sum_{i=2}^n 2i+d-1}{\sum_{i=2}^n 2i+d}} + \sqrt{\frac{1}{2}} \right] + \sqrt{\frac{\sum_{i=2}^n 2i+d-1}{(2i+1)[(\sum_{i=2}^n 2i)+d-2i]}}$$

Theorem 3.12. Let $Kg_{d,k}$ be the Kragujevac tree of degree $d \geq 2$, with branches B_k and the rooted trees $\beta_1, \beta_2, \dots, \beta_d \in B_{i+1}, B_{i+2}, \dots, B_{i+n}, \forall i = 1, 2, 3, \dots$, respectively. Then the third atom bond connectivity for $Kg_{d,k}$ is

$$ABC_3[Kg_{d,k}] = \sum_{i=2}^n i \left[\sqrt{\frac{\sum_{i=2}^n 2i+d-1}{\sum_{i=2}^n 2i+d}} + \sqrt{\frac{1}{2}} \right] + \sqrt{\frac{\sum_{i=2}^n 2i+d-1}{(2i+1)[(\sum_{i=2}^n 2i)+d-2i]}}$$

Proof. Let $Kg_{d,k}$ be the Kragujevac tree of degree $d \geq 2$, with branches $B_k, \forall k = 2, 3, \dots$, we consider here in particular rooted trees $[\beta_1, \beta_2, \dots, \beta_d]$ of the type $B_{i+1}, B_{i+2}, \dots, B_{i+n}, \forall i = 1, 2, 3, \dots$, respectively.

We consider the following cases to construct the ABC_3 of $Kg_{d,k}$.

Case i. By Remark 3.9, the branches $B_{i+1}, B_{i+2}, \dots, B_{i+n}$ has $(2[(i+1)+(i+2)+\dots+(i+n)])$ edges. In that $[(i+1)+(i+2)+\dots+(i+n)]$ edges are incident with pendent vertices and vertices of degree 2. Further one edge is closer to the pendent vertices and $(2[(i+1)+(i+2)+\dots+(i+n)]+d)$ edges are closer to the vertices of degree 2.

Case ii. The remaining $[(i+1)+(i+2)+\dots+(i+n)]$ edges of branch B_k are incident with vertices of degree 2 and vertices of degree $[(i+1)+1, (i+2)+1, \dots, (i+n)+1]$ respectively. Further 2 edges are closer to the vertices of degree 2 and $(2[(i+1)+(i+2)+\dots+(i+n)]+d-1)$ edges are closer to the vertices of degree $[(i+1)+1, (i+2)+1, \dots, (i+n)+1]$.

From equation (3),

$$ABC_3 = \sum_{i=2}^n i \left[\sqrt{\frac{\sum_{i=2}^n (2i)+d-1}{\sum_{i=2}^n (2i)+d}} + \sqrt{\frac{1}{2}} \right] \quad (17)$$

Case iii. Now consider the remaining d edges of $Kg_{d,k}$ which are incident with vertex of degree d and the vertices of degree $[(i+1)+1, (i+2)+1, \dots, (i+n)+1]$ belongs to the branches $B_{i+1}, B_{i+2}, \dots, B_{i+n}$ respectively. Also $(2i+1), (2i+2), \dots, (2i+n)$ vertices are closer to the vertices of degree $(i+1)+1, (i+2)+1, \dots, (i+n)+1$ respectively and $(\sum_{i=2}^n 2i)+d-2(i+1) (\sum_{i=2}^n 2i)+d-2(i+2) \dots, (\sum_{i=2}^n 2i)+d-2(i+n)$ vertices are

1), $(2i+2), \dots, (2i+n)$ edges are closer to the vertices of degree $(i+1)+1, (i+2)+1, \dots, (i+n)+1$ respectively and $\left(\sum_{i=2}^n 2i\right) + d - 2(i+1), \dots, \left(\sum_{i=2}^n 2i\right) + d - 2(i+n)$ edges are closer to the vertex of degree d , when the vertex of degree d is adjacent with vertices of degree $(i+1)+1, (i+2)+1, \dots, (i+n)+1$ respectively.

From equation (3),

$$ABC_3 = \sum_{i=2}^n \sqrt{\frac{\sum_{i=2}^n (2i) + d - 1}{(2i+1)[\sum_{i=2}^n 2i] + d - 2i]} \quad (18)$$

From (17) and (18),

$$ABC_2[Kg_{d,k}] = \sum_{i=2}^n i \left[\sqrt{\frac{\sum_{i=2}^n 2i + d - 1}{\sum_{i=2}^n 2i + d}} + \sqrt{\frac{1}{2}} \right] + \sqrt{\frac{\sum_{i=2}^n 2i + d - 1}{(2i+1)[\sum_{i=2}^n 2i] + d - 2i}}$$

Theorem 3.13. Let $Kg_{d,k}$ be the Kragujevac tree of degree $d \geq 2$, with branches $B_{k'}$ and the rooted trees $\beta_1, \beta_2, \dots, \beta_d \in B_{i+1}, B_{i+2}, \dots, B_{i+n}, \forall i = 1, 2, 3, \dots$, respectively. Then the fourth atom bond connectivity for $Kg_{d,k}$ is

$$ABC_4[Kg_{d,k}] = \sum_{i=2}^n i \left[\sqrt{\frac{3i+d}{(i+2)(2i+d)}} + \sqrt{\frac{1}{2}} \right] + \sum_{i=2}^n \sqrt{\frac{\sum_{i=2}^n (i+1) + (2i+d) - 2}{(2i+d)[\sum_{i=2}^n (i+1)]}}$$

Proof. Let $Kg_{d,k}$ be the Kragujevac tree of degree $d \geq 2$, with branches $B_{k'}, \forall k' = 2, 3, \dots$, we consider here in particular rooted trees $[\beta_1, \beta_2, \dots, \beta_d]$ of the type $B_{i+1}, B_{i+2}, \dots, B_{i+n}, \forall i = 1, 2, 3, \dots$, respectively.

We consider the following cases to construct the ABC_4 of $Kg_{d,k}$.

Case i. By Remark 3.9, the branches $B_{i+1}, B_{i+2}, \dots, B_{i+n}$ has $(2[(i+1) + (i+2) + \dots + (i+n)])$ edges. In that $[(i+1) + (i+2) + \dots + (i+n)]$ edges are incident with pendent vertices and vertices of degree 2. For the pendent vertices the neighbor vertices are of degree 2 and for the vertices of degree 2 the neighbor vertices are of degree $(i+1)+2, (i+2)+2, \dots, (i+n)+2$ belongs to the branches $B_{i+1}, B_{i+2}, \dots, B_{i+n}$ respectively.

Case ii. Now consider the remaining $[(i+1) + (i+2) + \dots + (i+n)]$ edges of branch B_k are incident with vertices of degree 2 and vertices of degree $[(i+1)+1, (i+2)+1, \dots, (i+n)+1]$ respectively. For the vertices of degree 2 the neighbor are of degree $(i+1)+2, (i+2)+2, \dots, (i+n)+2$ belongs to the branches $B_{i+1}, B_{i+2}, \dots, B_{i+n}$ respectively and for the vertices of degree $(i+1)+1, (i+2)+1, \dots, (i+n)+1$ the neighbor vertices are of degree $2(i+1)+d, 2(i+2)+d, \dots, 2(i+n)+d$ respectively.

From equation (4),

$$ABC_4 = \sum_{i=2}^n i \left[\sqrt{\frac{3i+d}{(i+2)(2i+d)}} + \sqrt{\frac{1}{2}} \right] \quad (19)$$

Case iii. Lastly consider the remaining d edges of $Kg_{d,k}$ which are incident with vertex of degree d and the vertices of degree $[(i+1)+1, (i+2)+1, \dots, (i+n)+1]$ belongs to the branches $B_{i+1}, B_{i+2}, \dots, B_{i+n}$ respectively. For the vertex of degree d the neighbor vertices are of degree $(i+1)+1, (i+2)+1, \dots, (i+n)+1$ with respect to the branches $B_{i+1}, B_{i+2}, \dots, B_{i+n}$ and for the vertices of degree $(i+1)+1, (i+2)+1, \dots, (i+n)+1$ the neighbor vertices are of degree $2(i+1)+d, 2(i+2)+d, \dots, 2(i+n)+d$ respectively.

From equation (4),

$$ABC_4 = \sum_{i=2}^n \sqrt{\frac{\sum_{i=2}^n (i+1) + (2i+d) - 2}{(2i+d)[\sum_{i=2}^n (i+1)]}} \quad (20)$$

From (19) and (20),

$$ABC_4[Kg_{d,k}] = \sum_{i=2}^n i \left[\sqrt{\frac{3i+d}{(i+2)(2i+d)}} + \sqrt{\frac{1}{2}} \right] + \sum_{i=2}^n \sqrt{\frac{\sum_{i=2}^n (i+1) + (2i+d) - 2}{(2i+d)[\sum_{i=2}^n (i+1)]}}$$

DISCUSSION

The original atom bond connectivity index was introduced in 1990's and is defined in [2]. Atom bond connectivity Indices of Kragujevac trees emerged in several studies addressed to solve the problem of characterizing the tree with minimal atom bond connectivity index [5,13,14]. Let G be a simple graph on n vertices. By uv we denote the edge connecting the vertices u and v . A vertex of degree one is referred to as a pendent vertex. An edge whose one end vertex is pendent is referred to as a pendent edge. The formal definition of a Kragujevac tree was introduced in [18].

Hence by using degree of vertices, distances between the vertices and edges of Kragujevac tree, we established our results for atom bond connectivity indices of Kragujevac trees.

CONCLUSION

In this article, we studied the first four types of atom bond connectivity indices and have calculated the first four types of atom bond connectivity indices for Kragujevac trees with isomorphic branches and increased ordered branches. Also in this article we observe the second and third atom bond connectivity indices are same for Kragujevac trees for both isomorphic and increasing ordered branches. Nevertheless, there are still many other class of graphs that are not covered

here. For further research, the atom bond connectivity indices for other class of graphs can be computed.

ACKNOWLEDGEMENT

Authors acknowledge the immense help received from the scholars whose articles are cited and included in references of this manuscript. The authors are also grateful to authors / editors / publishers of all those articles, journals and books from where the literature for this article has been reviewed and discussed.

Conflict of Interest: Nil

Source of Funding: Nil

REFERENCES

1. S. J. Cyvin and I. Gutman, *Kekulé Structures in Benzenoid Hydrocarbons*, Lecture Notes in Chemistry, Springer Verlag, Berlin, 46, (1988).
2. E. Estrada, L. Torres, L. Rodríguez, I. Gutman, *An atom-bond connectivity index: modelling the enthalpy of formation of alkanes*, Indian J. Chem., 37A, (1998), 849–855.
3. M. R. Farahani, *Computing a New version of Atom bond connectivity Index of circumcoronene Series of Benzenoid H_k by using Cut Method*, J. Math. Nano Science, 2, (2012) (In press).
4. B. Furtula, A. Graovac and D. Vukićević, *Atom-bond connectivity index of trees*, Disc. Appl. Math. 157, (2009), 2828 - 2835.
5. B. Furtula, I. Gutman, M. Ivanović and D. Vukićević, *Computer search for trees with minimal ABC index*, Appl. Math. Comput., 219, (2012), 767 - 772.
6. M. Ghorbani, M. A. Hosseini, *Computing ABC_4 index of nanostar dendrimers*, optoelectron. Adv. Mater. - Rapid commun. 4(9), (2010), 1419 - 1422.
7. Graovac and M. Ghorbani, *A New version of Atom-Bond Connectivity Index*. Acta chim. Slov., 57, (2010), 609 - 612.
8. A. Graovac, I. Gutman and N. Trinajstić, *Topological Approach to the Chemistry of Conjugated Molecules*, Springer Verlag, Berlin, (1977).
9. A. Graovac, I. Gutman and D. Vukićević, Eds., *Mathematical Methods and Modelling for Students of Chemistry and Biology*, Hum naklada, Zagreb, (2003).
10. I. Gutman, *Graph Theory Notes New York*, 27, (1994), 9 - 15.
11. I. Gutman, *Kragujevac trees and their energy*, SER. A: Appl. Math. Inform. and Mech. 6(2), (2014), 71 - 79.
12. I. Gutman and A. R. Ashrafi, *The edge version of the Szeged Index*, Croat. Chem. Acta, 81, (2008), 263 - 266.
13. I. Gutman and B. Furtula, *Trees with smallest atom-bond connectivity index*, MATCH Commun. Math. Comput. Chem., 68, (2012), 131 - 136.
14. I. Gutman, B. Furtula and M. Ivanović, *Notes on trees with minimal atom-bond connectivity index*, MATCH Commun. Math. Comput. Chem., 67, (2012), 467 - 482.
15. I. Gutman and O. E. Polansky, *Mathematical concepts in organic chemistry*, Springer Verlag, Berlin, (1986).
16. F. Harary, *Graph Theory*, Addison - Wesely, Reading, (1969).
17. H. Hosoya, *On Some Counting Polynomials in Chemistry* Disc. Appl. Math., 19, (1988), 239 - 257.
18. S. A. Hosseini, M. B. Ahmadi and I. Gutman, *Kragujevac Trees with minimal Atom-bond Connectivity Index*, MATCH Commun. Math. Comput. Chem., 71, (2014), 5 - 20.
19. P. V. Khadikar, S. Karmarkar and V. K. Agrawal, *A novel PI index and its applications to QSPR/QSAR studies*. J. chem. Inf. Comput. Sci., 41, (2001), 934 - 949.
20. N. Raos and A. Milićević, *Topological indices in estimating coordination compound stability constants*, Arh. Hig. Rada Toksikol., 60, (2009), 123 - 128.
21. N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, FL, (1992).
22. N. Trinajstić and I. Gutman, *Mathematical Chemistry*, Croat. Chem. Acta, 75, (2002), 329 - 356.
23. T. S. Vassilev, L. J. Huntington, *On the minimum ABC index of chemical trees*, J. Appl. Math. 2, (2012), 8 - 16.
24. H. Wiener, *Structural determination of paraffin boiling points*, J. Am. Chem. Soc., 69, (1947), 17 - 20.
25. R. Xing, B. Zhou, *Extremal trees with fixed degree sequence for atom-bond connectivity index*, Filomat, 26, (2012), 683 - 688.
26. R. Xing, B. Zhou, Z. Du, *Further results on atom-bond connectivity index of trees*, Discr. Appl. Math. 158, (2011), 1536 - 1545.
27. J. Yang, F. Xia, H. Cheng, *The atom-bond connectivity index of Benzenoid systems and phenylenes*, Int. Math. Forum, 6, (2011), 2001 - 2005.